Coulomb Blockade with Dispersive Interfaces

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What quantity controls the Coulomb blockade oscillations if the dot–lead conductance is essentially frequency–dependent? We argue that it is the *ac dissipative* conductance at the frequency given by the effective charging energy. The latter may be very different from the bare charging energy due to the interface–induced capacitance (or inductance). These observations are supported by a number of examples, considered from the weak and strong coupling (perturbation theory vs. instanton calculus) perspectives.

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The quantum fluctuations of charge in a Coulomb blockade (CB) quantum dot [1, 2] have been a subject of intense studies (see Refs. [3, 4] for a recent review). It is widely accepted that the dimensionless (in units of $G_Q = e^2/(2\pi\hbar)$) conductance, G, of the interface between the dot and a lead controls the strength of the quantum fluctuations. If G < 1 (weak coupling) the fluctuations are small (possibly apart from the degeneracy points) and usually may be accounted for by the perturbation theory in G [4, 5, 6]. On the other hand, for G > 1 (strong coupling) the CB is basically destroyed by the fluctuations. The remained weak CB oscillations may be described in the instanton approach [7, 8, 9, 10, 11, 12].

What happens if the conductance of the interface is essentially frequency–dependent, $G = G(\omega)$? Is it the dc conductance, G(0), or rather an ac one, $G(\Omega_c)$, (or may be none of them) that governs the strength of the quantum fluctuations? Is there a single parameter that divides the regions of applicability of the perturbation theory and the instanton calculations? What energy scale controls the thermal fluctuations? These are the questions we address in the present paper [13].

We argue that it is the dissipative ac conductance, $\Re e\,G(\Omega_c)$, that controls the quantum fluctuations and seamlessly divides between the two methods of description. The relevant frequency Ω_c has the meaning of an effective charging energy of the dot, $\Omega_c \sim e^2/(C + \tilde{C})$, where C is the bare capacitance of the dot and $\tilde{C}(\omega)$ is the parallel capacitance induced by the dispersive interface. Frequency Ω_c is the solution of the following self–consistent equation:

$$G_Q^{-1}\left(C + \tilde{C}(\Omega_c)\right) = \Omega_c^{-1}; \quad \tilde{C}(\omega) \equiv G_Q \,\partial_\omega G(i\omega).$$
 (1)

The effective charging energy, Ω_c , serves also as the characteristic scale for the thermal smearing of the CB. The induced capacitance, $\tilde{C}(\omega)$, is not necessarily positive and therefore Ω_c may be on the either side of the bare charging energy, $E_c = e^2/(2C)$.

To illustrate these points we consider three specific examples. In one of them (tunnelling barrier): $G(0) \approx G(\Omega_c)$. In the second (resonant impurity interface) the

dc conductance is parametrically larger than the ac one, $G(0) \gg G(\Omega_c)$. Finally, in the third example (shallow 2d lead) the situation may be reversed: $G(0) \ll G(\Omega_c)$. We treat all the examples from both weak and strong coupling perspectives. While the former is relatively straightforward, the latter requires certain technical adjustments to the way the instanton calculus is usually applied to the CB problem.

The CB is described by the following partition function

$$Z(q) = \sum_{W = -\infty}^{\infty} e^{i2\pi qW} \int_{\phi(\beta) - \phi(0) = 2\pi W} \mathcal{D}\phi \ e^{-S[\phi]} \ , \qquad (2)$$

where q is the external charge controlled by the gate voltage and W are integer winding numbers [2]. The imaginary time phase action has the form [14]

$$S[\phi] = \int_{0}^{\beta} d\tau \, \frac{\dot{\phi}^{2}(\tau)}{4E_{C}} - \iint_{0}^{\beta} d\tau d\tau' \, e^{i\phi(\tau)} K(\tau - \tau') e^{-i\phi(\tau')} \,.$$
(3)

The boson Matsubara transform $K(\omega_m) = K_m$ of the kernel $K(\tau)$ is given by

$$K_m = \text{Tr} \frac{1}{\beta} \sum_{\epsilon_n} \hat{\mathcal{W}}_n \mathcal{G}_n^{(l)} \hat{\mathcal{W}}_n^{\dagger} \left\{ \mathcal{G}_{n+m}^{(d)} - \mathcal{G}_n^{(d)} \right\} , \qquad (4)$$

where $\hat{W}_n = \hat{W}(\epsilon_n)$ is the tunnelling matrix connecting the dot and the lead and $\mathcal{G}_n^{(d,l)} = \mathcal{G}^{(d,l)}(\epsilon_n)$ are the fermion Green functions of the dot and lead correspondingly. The linear ac conductance of the interface is determined by the kernel, K_m . Indeed, employing the Kubo formula, one finds for the Matsubara transform of the conductance $G_m = -4\pi |\omega_m|^{-1} \Re e \, K_m$. After analytical continuation from the upper complex half-plane, $\omega_m \to -i\omega$, one obtains the complex ac interface conductance $G(\omega)$. The kernel K_m is also related to the non-linear current-voltage characteristic of the interface [15]. Namely, $I(V) = 2e \Im \{K|_{\omega_m \to ieV}\}$ is the current through the interface, provided that the voltage V is applied across it. We shall mostly employ the ac interpretation, although the I-V language is also possible.

In the weak coupling regime one expands $\exp\{-S[\phi]\}$ in the power series over the K-term in Eq. (3). Performing then the Gaussian ϕ -integration and W-summation, one finds for the average number of electrons on the dot, $\delta N(q) \equiv q + (2\beta E_c)^{-1} \partial \ln Z/\partial q$:

$$\delta N(q) = \int_{-\infty}^{\infty} d\tau \, \tau K(\tau) \, e^{-E_C(|\tau| - 2q\tau)} \,. \tag{5}$$

We have restricted ourselves to the temperature range $\beta E_C > 1$ and thus extended the integration to infinity. For a closed dot the electron number stays constant for |q| < 1/2 and jumps by one at the degeneracy points, $q = \pm 1/2$. A weak coupling, $K(\tau)$, makes the electron number to change smoothly in between the degeneracy points. It is clear from Eq. (5) that, apart from the immediate vicinity of $q = \pm 1/2$ [16], it is the short time, $|\tau| < E_c^{-1}$, behavior of $K(\tau)$ that determines $\delta N(q)$. One expects, thus, Eq. (5) to be valid if $\Omega_c \approx E_c$ and $\Re e G(\Omega_c) \ll 1$.

If this is not the case one may employ the instanton approach. To this end one has to find stationary configurations of the action (3) with a fixed winding number, e.g. W=1. We are unable to execute this program for an arbitrary $K(\tau)$ and employ instead the variational method. As a trial variational solution we take a family of Korshunov instantons [17]:

$$e^{i\phi(\tau)} = \frac{e^{2\pi i\tau/\beta} - z}{1 - e^{2\pi i\tau/\beta}z^*} , \qquad (6)$$

where z is a complex number with |z| < 1 that determines location and the width of the instanton. The action of a trial configuration is, in general, complex. Its imaginary part is simply a shift of the background charge, q, which affects only a phase of the CB oscillations. Hereafter we focus on the real part. Substituting the trial phase configuration, Eq. (6), into Eq. (3), one finds

$$\Re e S(\Omega) = \frac{\pi \Omega}{2E_c} + \frac{\pi \partial}{\partial (\beta \Omega)} \sum_{m=0}^{\infty} \left(1 - \frac{2\pi}{\beta \Omega} \right)^m G(\omega_m), \quad (7)$$

where $\beta\Omega/(2\pi) \equiv (1-|z|^2)^{-1} \geq 1$ is the inverse width of the instanton. One should minimize now $Z_1 \sim (\beta\Omega) \exp\{-\Re e \, S(\Omega)\}$ with respect to the instanton width, Ω^{-1} . The factor $\beta\Omega$ originates from the integration over the zero mode associated with the instanton location, $\arg z$. The minimum is reached at $\Omega = \Omega_c$ that is a solution of the stationary point equation $d\Re e \, S(\Omega)/d\Omega = \Omega^{-1}$. At low temperature this equation essentially coincides with Eq. (1). The optimal instantons are usually narrow, $\beta\Omega_c \gg 1$, that justifies the noninteracting instanton gas approximation. Summing up the gas of optimal instantons and anti-instantons [8, 12], one finds for the average number of electrons

$$\delta N(q) = q - c \frac{\Omega_c}{E_c} e^{-\Re e S(\Omega_c)} \sin(2\pi q + \varphi); \qquad (8)$$

with a model dependent proportionality coefficient, c, and phase, φ . This result is applicable if $\Re e S(\Omega_c) \gg 1$.

We have also employed the trial configuration of the form $\phi(\tau) = 4\arctan\left(\exp\{\Omega\tau\}\right)$, that is known to be a solution for the Josephson tunnelling problem [18]. The results differ from those obtained with Eq. (6) only by numerical coefficients. That makes us believe that our variational approach is parametrically accurate. We turn now to the applications of these results for the specific examples.

- (i) Frequency-independent conductance: $G_m = G_0$. This is the case e.g. if both lead and dot have continuous spectrum, $\mathcal{G}_n^{(d,l)} = i\pi\nu^{(d,l)}\operatorname{sign}(\epsilon_n)$, and energy independent tunnelling matrix elements, \mathcal{W} . In the low temperature limit the kernel has the form $K(\tau) = G_0/(2\pi\tau)^2$. Employing Eq. (5), one finds for a weakly coupled dot [5] $\delta N(q) = \frac{G_0}{(2\pi)^2} \ln \frac{1+2q}{1-2q}$. In the strong coupling regime the trial phase, Eq. (6), is the exact solution of the saddle point equation. For $\Omega \ll E_c$ the action $\Re e S(\Omega) = G_0/2$ is Ω -independent. As a result, there is an additional zero mode associated with the instanton width. presence of such zero-mode complicates calculations of the pre-exponential factor. We quote here only the result [8, 11, 12]: $c\Omega_c$ in Eq. (8) must be substituted by $(2\pi)^{-1}E_cG_0^2\ln(\beta E_c)$. The additional zero-mode leads to the instanton-instanton interactions that break the noninteracting instanton gas approximation at temperature $\beta^{-1} \approx E_c G_0^2 \exp\{-G_0/2\}$. At smaller temperature the amplitudes of the higher q-harmonics are probably of the same order as the first one. That may lead to a nonanalytic behavior at the degeneracy points, $q = \pm 1/2$, in the zero temperature limit, similar to that of Ref. [19]. As expected, the unit conductance, $G_0 \approx 1$, separates the strong and weak coupling regimes.
- (ii) Resonant impurity. Consider an interface where the particle exchange between the dot and bulk takes place only through resonant impurity levels. For a single channel this model was solved in Ref. [20]. We shall assume for simplicity that all the levels are at the Fermi energy and have the same coupling to the bulk (width), $\Gamma \ll E_c$. The Green function of the lead is given by that of the resonant impurity level: $\mathcal{G}_n^{(l)} = (i\epsilon_n + i\Gamma \text{sign}(\epsilon_n))^{-1}$. With the help of Eq. (4), one finds for the kernel:

$$K_m = -\frac{G_0 \Gamma}{4\pi} \ln \left(1 + \frac{|\omega_m|}{\Gamma} \right) . \tag{9}$$

Accordingly the linear conductance takes the form $G(\omega) = G_0 \Gamma i \omega^{-1} \ln(1 - i\omega/\Gamma)$, where G_0 is the dc resonant conductance proportional to the number of impurities and their coupling to the dot [21]. The short time, $\Gamma \tau \ll 1$, limit of the kernel is $K(\tau) = G_0 \Gamma/(8\pi|\tau|)$. Employing Eq. (5), one obtains for $\delta N(q)$ not too close to the degeneracy points, $q = \pm 1/2$ [20]:

$$\delta N(q) = \frac{G_0 \Gamma}{8\pi E_c} \left(\frac{1}{1 - 2q} - \frac{1}{1 + 2q} \right). \tag{10}$$

Notice, that the criterion of the weak coupling is $G_0\Gamma/E_c\ll 1$ [20], while the dc conductance, G_0 , may be large. In such a case Eq. (1) is solved by $\Omega_c\approx E_c$. Since $\Re e\,G(\omega)=\pi G_0\Gamma/(2\omega)$ for $\omega\gg\Gamma$, one finds that $\delta N(q)\sim \Re e\,G(\Omega_c)$. As a result, the weak coupling approximation is valid as long as $\Re e\,G(\Omega_c)\ll 1$.

In the strong coupling regime, employing Eq. (7), one finds for the variational action

$$\Re e \, S(\Omega) = \frac{\pi \Omega}{2E_0} + \frac{G_0 \Gamma}{2\Omega} \, e^{\Gamma/\Omega} E_1 \left(\Gamma/\Omega \right) \,, \tag{11}$$

where E_1 is the exponential integral. This action possess two stationary points as a function of the instanton width, Ω^{-1} . One is the stable minimum at $\Omega_c = \sqrt{G_0 \Gamma E_c/(2\pi)} \ln^{1/2}(G_0 E_c/\Gamma)$, with the action $\Re e \, S(\Omega_c) = \pi \Omega_c/E_c$. The other is the unstable plateau at $\Gamma\Omega^{-1} > 1$ with the action given by half of the dc conductance: $\Re e \, S(0) = G_0/2$, in agreement with (i). One may check that Ω_c is indeed the solution of Eq. (1). Up to logarithmical factor [22], $\Re e \, S(\Omega_c) \approx \Re e \, G(\Omega_c)$ and the condition $\Re e \, G(\Omega_c) \approx \sqrt{G_0 \Gamma/E_c} \gg 1$ justifies validity of the instanton approach.

At not very small temperature, the stable minima at Ω_c (narrow instanton) is the only relevant one and the electron number is given by Eq. (8). The contribution of the wide instantons with $\Omega < |\tilde{\Gamma}|$ is exponentially smaller $\sim G(0)^2 \ln(\beta|\tilde{\Gamma}|) e^{-G(0)/2}$ and may be disregarded as long as $G(0) \gg \Re e G(\Omega_c) \approx \Re e S(\Omega_c)$. Nevertheless, due to the phenomena mentioned in (i), the wide instantons may prove to be important in an immediate vicinity of the degeneracy points and at very small temperature, $\beta^{-1} < E_c G_0^2 \exp\{-G(0)/2\}$. If so, then G(0), rather than $\Re e G(\Omega_c)$, controls the CB in that narrow range.

On the high temperature side the CB oscillations are washed out at $T > \Omega_c$. Notice, that in the strong coupling regime $\Omega_c > E_c$ and therefore the (weak) CB, Eq. (8), is more "temperature–tolerant" than in the weak coupling. The reason is that the induced capacitance, \tilde{C} , is negative (it is actually an inductance) and thus the effective charging energy is increased.

(iii) Shallow 2d lead. Consider a quantum dot coupled through a tunnelling barrier to a shallow 2d gas. The bottom of the 2d conductance band is at energy ε_0 below $(\varepsilon_0 < 0)$ or above $(\varepsilon_0 > 0)$ of the dot's Fermi energy. In the former case the dc conductance between the dot and 2d gas is given by the product of their densities of states and the tunnelling matrix elements and is denoted by G_0 . In the latter case the dc conductance is zero. We shall examine the effect of the proximity to such a lead $(\varepsilon_0 \ll E_c$ hereafter) on the CB in the dot.

The straightforward calculation yields for the coupling kernel:

$$K(\tau) = \frac{G_0}{(2\pi\tau)^2} \begin{cases} 1 - \theta(-\tau) e^{-\varepsilon_0 \tau}, & \varepsilon_0 < 0; \\ \theta(\tau) e^{-\varepsilon_0 \tau}, & \varepsilon_0 > 0. \end{cases}$$
(12)

The corresponding conductance, $G(\omega)$, obeys the symmetry relation $G_{-}(\omega) = G_{0} - G_{+}(\omega)$, where the subscripts

 \pm denote the sign of ε_0 . In the small temperature limit, $\beta \varepsilon_0 \gg 1$ one finds for the dissipative conductance

$$\Re e \, G_{+}(\omega) = \frac{G_0}{2} \, \theta(|\omega| - \varepsilon_0) \left(1 - \frac{\varepsilon_0}{|\omega|} \right) \,. \tag{13}$$

Notice, that $\Re e G(\omega) = 0$ for $|\omega| \leq \varepsilon_0$ if the 2d band is empty, $\varepsilon_0 > 0$. On the other hand, in the high frequency limit, $\omega \gg |\varepsilon_0|$, $\Re e G(\omega) = G_0/2$ irrespective to the sign of ε_0 . For the reactive conductance one obtains $\Im G_+(\omega) = G_0/(2\pi)f(|\omega|/\varepsilon_0)$, where we denoted $f(x) = \ln|x-1| - \ln|x+1| - x^{-1} \ln|x^2 - 1|$.

In the weak coupling limit, employing Eqs. (5) and (12), one finds for the average number of electrons:

$$\delta N(q) = \frac{G_0}{(2\pi)^2} \begin{cases} \ln \frac{1+2q}{1-2q} - \ln(1+|\varepsilon_0|/E_c + 2q), & \varepsilon_0 < 0; \\ -\ln(1+\varepsilon_0/E_c - 2q), & \varepsilon_0 > 0 \end{cases}$$
(14)

subtracted an irrelevant constant $-(G_0/(4\pi)^2) \ln \Lambda/E_c$, where Λ is the 2d band-width). For the shallow filled 2d gas ($\varepsilon_0 < 0$) the result is only slightly different from (i). Surprisingly, for the empty 2d band ($\varepsilon_0 > 0$) one finds a q-dependence of δN , despite of the fact that the dc conductance is strictly zero. This dependence is parametrically similar to that of the filled 2d gas, however does not exhibit singularities, indeed |q| < 1/2. It is associated with the virtual transitions between the dot and the empty 2d band. Since $\varepsilon_0 \ll E_c$, such transitions are possible and the coupling strength is determined by G_0 only. For $G_0 < 1$ Eq. (1) is solved by $\Omega_c \approx E_c$. The applicability of the weak coupling approximation is therefore controlled by the condition $\Re e G(\Omega_c) = G_0/2 \ll 1 \text{ (and } not \ G(0) \ll 1 \text{ !)}.$

We shall approach now the problem from the strong coupling perspective. To this end we employ the variational expression, Eq. (7). For $\varepsilon_0 < 0$ the variational action is $\Re e \, S = G_0(1 - \Omega/(\pi \varepsilon_0))/2$ for $\Omega \ll |\varepsilon_0|$, while it approaches $\Re e \, S = G_0/4 + \pi \Omega/E_c$ for $\Omega \gg |\varepsilon_0|$. There is a broad minimum at $|\varepsilon_0| \ll \Omega_c < E_c$. As a result, $\Re e \, S(\Omega_c) = G_0/4$ and the electron number is given by Eq. (8) (possibly apart from the immediate vicinity of $q = \pm 1/2$). This result is valid for $\Re e \, G(\Omega_c) = G_0/2 \gg 1$.

For the empty 2d band, $\varepsilon_0 > 0$, the variational action is $\Re e \, S = G_0 \Omega/(2\pi\varepsilon_0)$ for $\Omega \ll \varepsilon_0$ and riches $G_0/4$ at $\varepsilon_0 \ll \Omega < E_c$. Naively, it has a minimum at $\Omega_c \to 0$ with $\Re e \, S(0) = 0$. One has to include, however, the fluctuation part into the stationary point equation, as discussed after Eq. (8). As a result, for $G_0 \gg 1$ one finds the stable extremum at $\Omega_c = 2\pi\varepsilon_0/G_0$. The corresponding electron number is $\delta N(q) = q - c\varepsilon_0/(G_0E_c)\sin(2\pi q)$. Despite being obtained in the instanton approach, the correction is not exponentially small. The formal reason is that $\Re e \, S(\Omega_c) = 1$, that makes the above result an order of magnitude estimate, at best. Fortunately, one can solve the problem in a different way.

As was shown above the "straight" instantons, $\phi_W(\tau) = 2\pi W \tau/\beta$, are the most stable. One can, thus,

calculate the partition function as a sum over such instantons. The action is the Matsubara transform of the kernel: $\Re e S[\phi_W] = -\beta \Re e K(\omega_W) \approx W^2 G_0/(2\beta \varepsilon_0)$. Employing Eq. (2), one finds $\ln Z(q) = -\beta q^2(2\pi^2 \varepsilon_0/G_0)$; valid at small temperature, $\beta^{-1} \ll \varepsilon_0/G_0$. As a result,

$$\delta N(q) = q \left(1 - \frac{2\pi^2 \varepsilon_0}{G_0 E_c} \right); \qquad |q| < 1/2 \qquad (15)$$

and there are small jumps by $\pi \varepsilon_0/(G_0 E_c) \ll 1$ at the degeneracy points $q = \pm 1/2$. The presence of such jumps could be anticipated from the absence of singularities in the weak coupling expression, Eq. (14).

Equation (15) states that there is a perfect CB with the reduced (screened) charging energy $\pi\Omega_c = 2\pi^2 \varepsilon_0/G_0$. Indeed, according to Eq. (1) the induced capacitance is given by $\tilde{C}(\omega) = e^2 G_0 \varepsilon_0 / (2\pi\omega)^2 \ln(1 + (\omega/\varepsilon_0)^2)$. As a result, one finds $\tilde{C} = e^2 G_0/(4\pi^2 \varepsilon_0) \gg C$ at small frequency, $\omega \ll \varepsilon_0$. The bare capacitance, C, appears to be completely screened and substituted by C. Solving Eq. (1) with such \tilde{C} , one obtains $\Omega_c = 2\pi\varepsilon_0/G_0$ that justifies the small frequency assumption, provided $G_0 \gg 1$. The amazing twist is that $\Re e G(\Omega_c) = 0$ and quantum fluctuations are practically absent. Therefore the larger G_0 is – the weaker is the coupling to the lead! By increasing G_0 one can restore the perfect CB with a very small charging energy, however. The (exponential) temperature smearing sets in at the temperature $\beta^{-1} \approx \Omega_c \ll E_c$, limiting an indefinite increase of G_0 .

Strictly speaking, the system is always in the weak coupling regime, $\Re e\,G(\Omega_c)\ll 1$ (possibly apart from $G_0\approx 1$). The perturbative result, Eq. (14), is valid, though, only for $G_0\ll 1$. For $G_0\gg 1$ Eq. (15) is to be employed. (It is in parametric agreement with the variational estimate, although the q-dependence of the latter is actually wrong.) The two results match at $G_0\approx 1$. Indeed, consider e.g. $\chi=\partial\delta N(q)/\partial q|_{q=0}$. For $G_0\ll 1$ one finds $\chi=(2\pi^2)^{-1}G_0/(1+\varepsilon_0/E_c)$, while for $G_0\gg 1$ $\chi=1-2\pi^2\varepsilon_0/(G_0E_c)$. Since $\varepsilon_0\ll E_c$, these two (weak coupling) expressions perfectly match at $G_0=2\pi^2$.

To summarize: we have argued that not too close to the degeneracy points the quantum fluctuations of charge are governed by the dissipative ac conductance $\Re e \, G(\Omega_c)$. The effective charging energy, Ω_c , has to be found as the solution of Eq. (1). It may substantially deviate from the bare charging energy, E_c , in either direction. For $\Re e \, G(\Omega_c) \ll 1$ and low enough temperature, $\beta \Omega_c \gg 1$, the charge on the dot is approximately quantized. Formally it stems from the fact that the large winding numbers, $W \approx \beta \Omega_c \gg 1$, give a dominant contribution to the partition function. In the opposite limit, $\Re e \, G(\Omega_c) \gg 1$, only the instantons with the smallest W's are important, while Ω_c acquires the meaning of the optimum inverse instanton width. In both cases for $\beta^{-1} > \Omega_c$ the thermal fluctuations smear the CB. On the other hand, very close

to the degeneracy points and at small temperature, the relevant parameter may prove to be the dc conductance, G(0). A detailed study of the last issue is beyond the scope of the present letter.

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